Biphenyl

92-52-4 | DTXSID4020161

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 17.6 days

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

Image not found
Biphenyl
Measured: 2720
Predicted: 17.6

Image not found
Naphthalene
Measured: 12.5
Predicted: 8.13

Image not found
1,2,4,5-Tetramethylbenzene
Measured: 88.3
Predicted: 5.46

Image not found
1,2,3,4-Tetramethylbenzene
Measured: 24.3
Predicted: 3.95

Image not found
Phenanthrene
Measured: 5460
Predicted: 75.9